

Problem 1: Starting a refinement with bad profile coefficients & only an approximate structure is quite hard

- Solution #1:
 - Collect data using a standard with a known structure
 - Fit the standard (easier since structure & cell can be fixed)
 - Create an instrument parameter file in INSTEDIT specific to the instrument type/conditions (CW only)

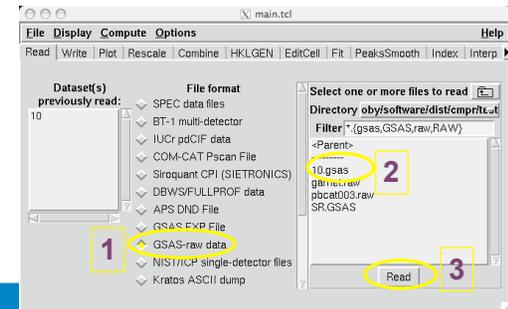
- Solution #2:
 - Fit peak widths for selected peaks (in CMPR or RAWPLOT)
 - Fit profile coefficients to peak widths (in CMPR) (CW only)
 - Edit profile terms in refinement or create/edit instrument parameter file in INSTEDIT

Will make use of CMPR program

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1.0 Peak fitting in CMPR. Step 1: Read in data

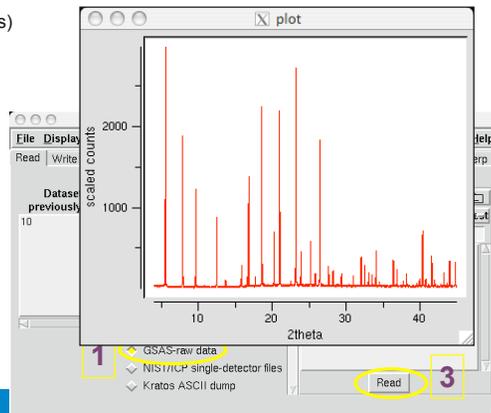
1. Select format
2. Select directory/file(s)
3. Push read button



1.1 Peak fitting in CMPR. Step 1: Read in data

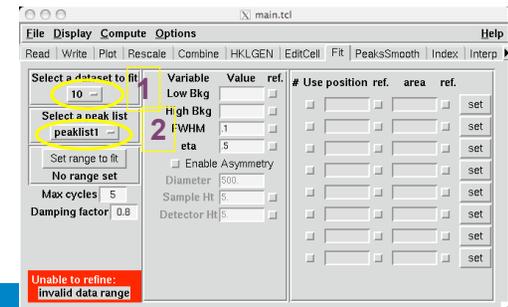
1. Select format
2. Select directory/file(s)
3. Push read button

Data then appear in plot window



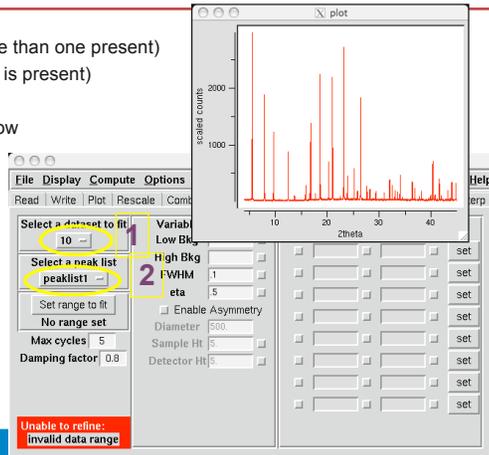
1.2a Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)



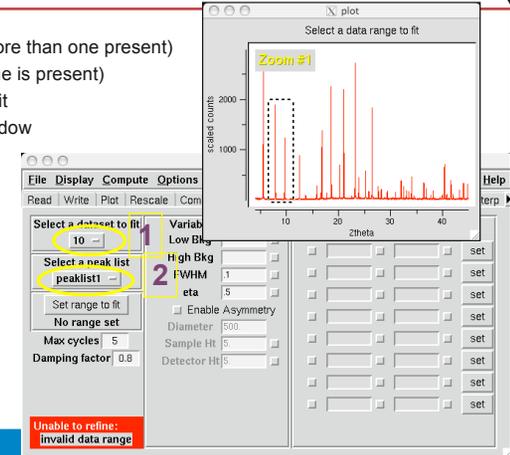
1.2b Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
 - Zoom in plot window



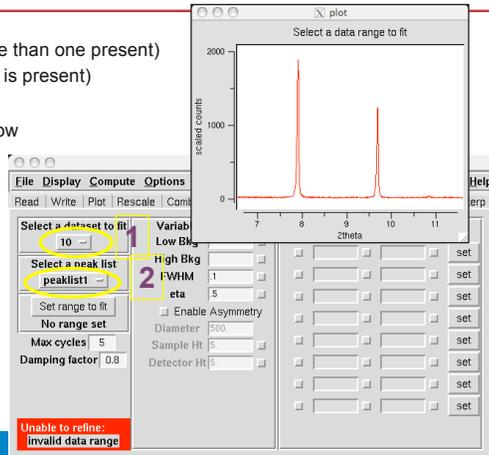
1.2c Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
 - Zoom in plot window



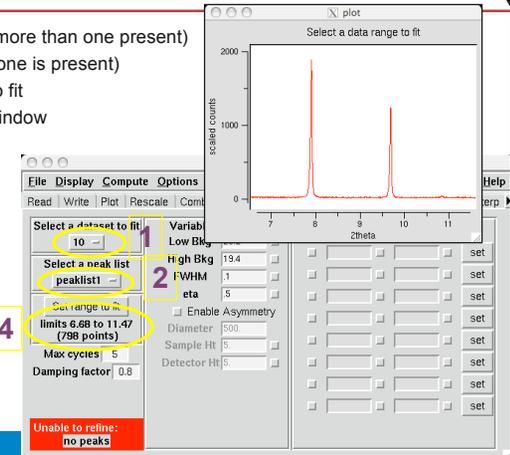
1.2d Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
 - Zoom in plot window



1.2e Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
 - Zoom in plot window
 - Press S key
4. Limits are shown



1.2f Peak fitting in CMPR. Step 2: Select range to fit

1. Select data set (if more than one present)
2. Select peak list (if one is present)
3. Set a data range to fit
 - Zoom in plot window
 - Press S key
4. Limits are shown

Note: step 3 can also be done using "Set Range" button

1.3a Peak fitting in CMPR. Step 3: Enter Peak Positions

1. Move mouse to peak location
2. Press P key

dataset to fit	Variable	Value	ref.	# Use position	ref.	area	ref.
10	Low Bkg	23.2					set
10	High Bkg	19.4					set
10	FWHM	1					set
10	eta	5					set
10	Enable Asymmetry						set
10	Diameter	500					set
10	Sample Ht	5					set
10	Detector Ht	5					set

1.3b Peak fitting in CMPR. Step 3: Enter Peak Positions

1. Move mouse to peak location
2. Press P key
 - a) line appears at peak location
 - b) Peak entry appears in table

Repeat for all peaks in section

dataset to fit	Variable	Value	ref.	# Use position	ref.	area	ref.
10	Low Bkg	23.2					set
10	High Bkg	19.4					set
10	FWHM	1					set
10	eta	5					set
10	Enable Asymmetry						set
10	Diameter	500					set
10	Sample Ht	5					set
10	Detector Ht	5					set

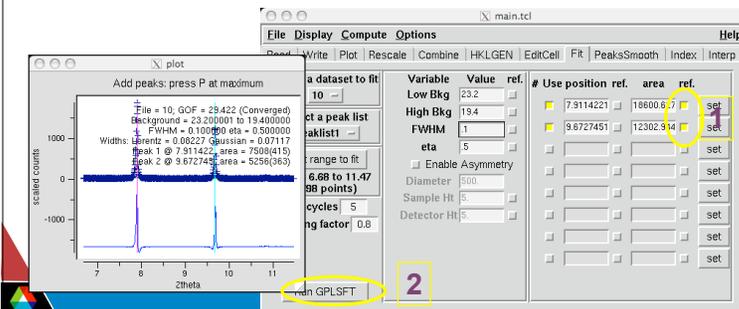
1.4a Peak fitting in CMPR. Step 4A: Start fitting peaks

1. Select peaks areas to be refined
2. Press run GPLS button to perform fit

dataset to fit	Variable	Value	ref.	# Use position	ref.	area	ref.
10	Low Bkg	23.2					set
10	High Bkg	19.4					set
10	FWHM	1					set
10	eta	5					set
10	Enable Asymmetry						set
10	Diameter	500					set
10	Sample Ht	5					set
10	Detector Ht	5					set

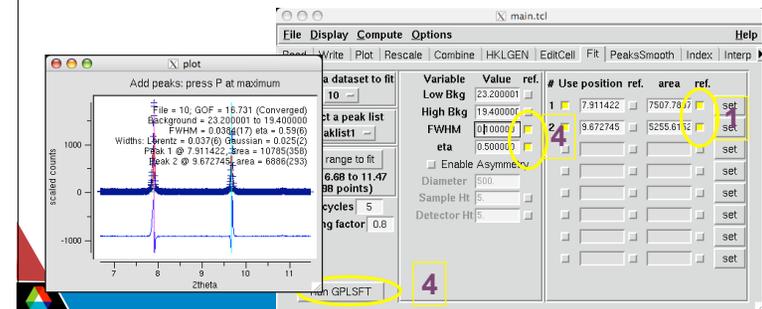
1.4b Peak fitting in CMPR. Step 4A: Start fitting peaks

1. Select peaks areas to be refined
2. Press run GPLS button to perform fit
3. Plot now shows [crummy] fit



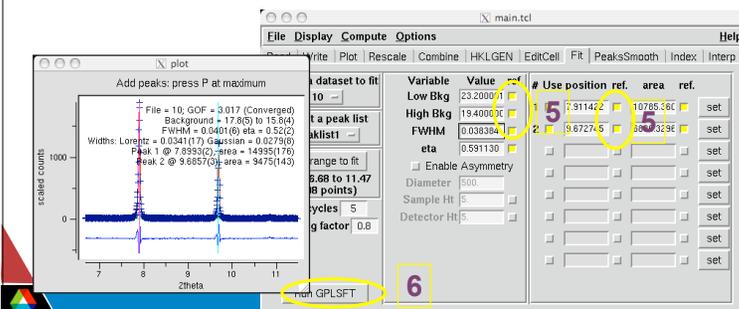
1.4c Peak fitting in CMPR. Step 4A: Start fitting peaks

1. Select peaks areas to be refined
2. Press run GPLS button to perform fit
3. Plot now shows [crummy] fit
4. Refine peak width & shape (Gaussian: eta = 0; Lorentz: eta = 1)



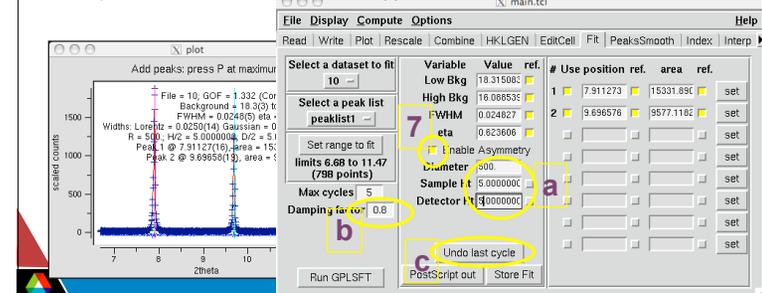
1.4d Peak fitting in CMPR. Step 4B: Continue fitting peaks

5. Select peaks positions & backgrounds to be refined in addition
6. Press run GPLS button to perform fit
7. Plot now shows reasonable fit



1.4e Peak fitting in CMPR. Step 4C: Treat Low-Angle Asymmetry (optional)

7. Turn on "Enable Asymmetry" & Refine
 - a) Don't refine sample & detector heights -- use measured value
 - b) If you have to refine heights; turn off other vars first and/or decrease damping
 - c) Also note "undo" button which appears after each refinement



1.4f Peak fitting in CMPR. Step 4D: Continue fitting peaks across pattern

8. Press "Set range to fit" button
 - a) Press Reset zoom
 - b) Zoom in on a new region to select a small number of peaks
 - c) Press "set from zoom" or the "S" key
9. Enter peaks & fit as before in steps 2-4

Fit peaks in >6 regions across pattern (>10 is better)

#	Pos	Gauss FWHM	Cauchy FWHM	Omit
1	7.911273	0.024627	0.02592	<input type="checkbox"/>
2	9.696576	0.02796	0.02608	<input type="checkbox"/>

1.5a Fit Profile Coefficients to Peak Widths in CMPR: Use FitWidths

1. Select peak list

1.5b Fit Profile Coefficients to Peak Widths in CMPR: Use FitWidths

1. Select peak list
2. Press "Fit Profile" button to fit UVW's

#	Pos	Gauss FWHM	Cauchy FWHM	Omit
1	5.92718	0.01645	0.024	<input type="checkbox"/>
2	7.911298	0.01406	0.02592	<input type="checkbox"/>
3	12.531071	0.01479	0.02796	<input type="checkbox"/>
4	15.864467	0.01551	0.02608	<input type="checkbox"/>
5	18.627426	0.01342	0.03107	<input type="checkbox"/>
6	21.037156	0.01433	0.03132	<input type="checkbox"/>
7	25.205482	0.0122	0.03937	<input type="checkbox"/>
8	25.838211	0.0122	0.03937	<input type="checkbox"/>
9	28.237577	0.01229	0.04547	<input type="checkbox"/>
10	28.803286	0.01229	0.04547	<input type="checkbox"/>

1.5c Fit Profile Coefficients to Peak Widths in CMPR: Use FitWidths

1. Select peak list
2. Press "Fit Profile" button to fit UVW's
3. Values from fitting appear in boxes; Plot shows fit
4. Write down U, V, W, X & Y values

#	Pos	Gauss FWHM	Cauchy FWHM	Omit
1	5.92718	0.01645	0.024	<input type="checkbox"/>
2	7.911298	0.01406	0.02592	<input type="checkbox"/>
3	12.531071	0.01479	0.02796	<input type="checkbox"/>
4	15.864467	0.01551	0.02608	<input type="checkbox"/>
5	18.627426	0.01342	0.03107	<input type="checkbox"/>
6	21.037156	0.01433	0.03132	<input type="checkbox"/>
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8	25.838211	0.0122	0.03937	<input type="checkbox"/>
9	28.237577	0.01229	0.04547	<input type="checkbox"/>
10	28.803286	0.01229	0.04547	<input type="checkbox"/>

1.6 Fitted Profile Coefficients in CMPR: Understanding the FitWidths Plot

- To label data on the plot
1. Use Display options in Options menu
 2. Select "Plot Legend" in plot options
 3. Plot now has legend

The screenshot shows the EXPGUI interface. The 'Options' menu is open, with 'Display options' selected. Below it, the 'Plot Legend' option is highlighted in the 'Plot options' section. The plot window shows a graph of intensity versus 2-theta with data points and fit lines. A legend in the bottom right corner identifies the data series: Gaussian (red circles), Cauchy (blue squares), Fit-Gaussian (red line), and Fit-Cauchy (blue line).

1.7a Start INSTEDIT from EXPGUI to modify an Instrument Parameter file

- There are two ways to start INSTEDIT:
- 1) from entry in Powder menu bar or

The screenshot shows the 'Powder' menu bar in EXPGUI. The 'instedit' option is visible at the bottom of the menu.

1.7b Start INSTEDIT from EXPGUI to modify an Instrument Parameter file

- There are two ways to start INSTEDIT:
- 1) from entry in Powder menu bar or
 - 2) Add New Histogram window

The screenshot shows the EXPGUI interface with the 'Add New Histogram' dialog box open. The 'Add New Histogram' button is highlighted with a yellow circle. The dialog box contains fields for 'Data file', 'Instrument Parameter file', and 'Select set'.

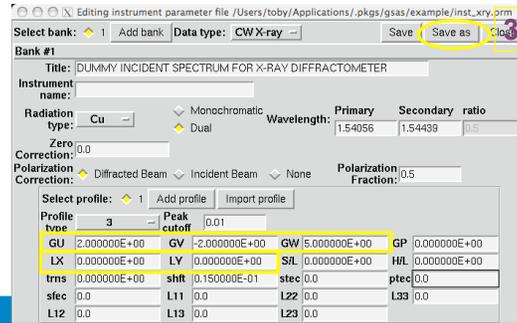
1.7c Start INSTEDIT from EXPGUI to modify an Instrument Parameter file

- There are two ways to start INSTEDIT:
- 1) from entry in Powder menu bar or
 - 2) Add New Histogram window
 - 3) Select instrument parameter file to start from
 - 4) Press Edit file to open INSTEDIT

The screenshot shows the 'Adding a new histogram' dialog box. The 'Select File' and 'Edit file' buttons are highlighted with yellow circles. The dialog box contains fields for 'Data file', 'Instrument Parameter file', and 'Select set'.

1.8 Use INSTEDIT to modify Instrument Parameter file contents

- 1) Set U,V & W as GU, GV & GW and X & Y as LX & LY; set GP = 0
- 2) While you are at it, set wavelength, S/L & H/L etc... to default values
- 3) Save under a new name



1.9 WIDPLT Tool in EXPGUI Can Be Used to Plot Peak Widths vs 2θ and Compare to Instrumental Resolution

- WIDPLT is EXPGUI Graphs menu

Reference widths are saved in files named widplt_...

Define a few items in this file for each reference:

```
set UVWP(Cu16) {289.7 -298.2 180.8 0}
set wave(Cu16) 1.54
set XY(Cu16) {0 0}
set lblarr(Cu16) "BT-1 Cu(311) 15"
set ttrange(Cu16) "5 165"
lappend datalist Cu16
```

(see file example_widplt_BT1)

